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MODELING EXPOSURE TO ELECTROMAGNETIC FIELDS WITH REALISTIC ANATOMICAL MODELS: THE BROOKS FINITE DIFFERENCE TIME DOMAIN (FDTD)

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Modeling Exposure to Electromagnetic Fields with Realistic Anatomical Models: The Brooks Finite Difference Time Domain (FDTD)

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ABSTRACT

Air Force Research Laboratory/Human Effectiveness Directorate Radio Frequency Radiation Branch (AFRL/RHDR) and Naval Health Research Center (NHRC) have long used Finite Difference Time Domain (FDTD) software to study radiofrequency radiation (RF) bioeffects. FDTD is a direct time-domain solver for Maxwell's equations. The original Brooks FDTD code was developed as part of the Brooks Dosimetry Project and has been repeatedly enhanced to meet empirical and theoretical research needs. Many feature upgrades have been added to the original Fortran FDTD code, and recently the code has been completely rewritten in C. Both versions of Brooks FDTD are parallelized for Beowulf clusters and have run on more than one hundred processors. In addition to code, a number of segmented anatomical models have been created for the Brooks Dosimetry Project. These models include a human, rhesus monkey, goat, and several rat models (See Appendix E). The Brooks FDTD codes, used with these anatomical models, allow researchers to perform useful RF bioeffects modeling to aid ongoing RHDR and NHRC research efforts. To ensure fidelity of FDTD results, Brooks FDTD has been validated using several methods which are reported here.

ACKNOWLEDGMENTS

Through the course of the development of these tools the Brooks Dosimetry Project has had a number of participants, advocates, and users both within the Department of Defense and in the scientific community. In particular, William Hurt and Patrick Mason with John Ziriax made the initial effort to establish a radio frequency computational modeling effort at Brooks. In additional, others who have made significant contributions include: Aldon Lyssy, who volunteered to scavenge and build the first Beowulf: Peter Gajsek who lead the first purely modeling project for his dissertation; and finally, to the numerous unknown "painter" whose tireless efforts to manually segment the anatomical models provided the essential "RAW" data for the project.

OVERVIEW

Background

The Finite Difference Time Domain (FDTD) method is a direct time-domain numerical approach for solving Maxwell's equations. The FDTD method was first introduced by Kane Yee in 1966 [1], and has become increasingly popular for electromagnetic modeling and simulation (M&S) as computational resources have increased.

The FDTD method is used for many types of applications, including military technology, radar systems, communication devices, computer circuit design, and studying the biological effect of exposure to electromagnetic (EM) energy.

Two FDTD codes have been written at Brooks; one implemented in Fortran [2] and one in C [3]. These codes have been used as part of a number of research projects studying the bioeffects of electromagnetic (EM) energy. Specifically, the code has been used to predict energy absorption rates within biological tissues due to incident fields in the radio frequency region of the EM spectrum.

An FDTD simulation is run by executing a command line directing the program to use basic text configuration files, command line options, and a binary model file. Upon completion of a simulation the program will output a binary result file containing the specific absorption rate (SAR) at each voxel of the anatomical model. SAR is a measure of the maximum rate at which RF energy is absorbed by the body when exposed to radio frequency electromagnetic fields. The maximum E-field can also be obtained in binary format depending upon options selected.

Due to the size of high resolution anatomical models and the large memory requirements for the FDTD algorithm, generally simulations exceed the capacity of a single workstation. Therefore, Brooks FDTD has been parallelized using Message Passing Interface (MPI) to distribute the problem over multiple processors. The software was designed to run on a Linux Beowulf cluster, which is advantageous because it allows the code to run on commodity hardware and free and open-source software. When a simulation is initiated, the model space is divided along the z-axis, which the longest axis for the anatomical models. Equal shares of the problem are then allocated to each processor for the simulation.

Objectives

The Brooks FDTD is used to calculate the SAR within realistic digital anatomical models. These simulations have allowed for the study of a much broader range of frequencies than would be possible by experimentation alone. SAR predictions have proven useful in experimental design, and in setting safety standards for EM fields.

These standards are essential for protecting the health and safety of the public as well as those working in a controlled environment.

The usefulness of Brooks FDTD is contingent upon its ability to produce results within an acceptable range of accuracy. Therefore, in addition to creating FDTD codes, we must also validate FDTD results with as many methods as possible. The purpose of this report is to document the validation efforts that have been completed for this software, as well as to provide a reference manual for the proper use of the code. Validation testing is presented in the Results and Discussion section.

Approach

Brooks FDTD was initially developed to model more complex geometries than possible with other existing models. We will compare both Brooks FDTD implementations against a Mie theory based code. Mie theory is a complete analytical solution for solving Maxwell's equations for the scattering of a plane wave on a sphere and is generally considered perfectly accurate since it is a closed form analytical solution. If the FDTD results approach the Mie values within an acceptable margin of error, we may assume the FDTD results are accurate within that margin of error.

Introduction

As directed energy (DE) technologies become more pervasive in DoD communications and weapon systems, it becomes critically important to understand associated bioeffects. AFRL/RHDR works in integrated teams including researchers from the Navy and Army, as well as Joint Non-Lethal Weapons Directorate Programs. This tri-service team provides bioeffects research of the entire electromagnetic spectrum covering lasers to radio frequency (RF). Tri-service DE bioeffects research plays an important role in developing world-wide safety standards for radio frequency and lasers.

Modeling and simulation provides a powerful tool for research in the areas of DE bioeffects. The tri-services team jointly developed and enhanced finite difference time domain (FDTD) codes for solving Maxwell's electromagnetic equations derived from Lawrence Livermore National Lab's original FDTD code [4] and the implementation presented by Kunz and Luebbers [5]. The Brooks FDTD code was created specifically to calculate the specific absorption rate of biological tissues exposed to RF. The code was validated by comparison to experimental results and known analytical solutions within geometrically simple models. This code was parallelized at Brooks and has been run for over four years on a Beowulf cluster. Modeling realistic anatomical digital models allowed researchers to predict areas of local energy deposition within the human body before actual experimentation, thereby improving the experimental design process. Modeling allows researchers to simulate a much wider range of frequencies, pulses, and sources than previously attained by experimentation alone due to time and funding constraints.

Background

The Finite Difference Time Domain (FDTD) is a direct time-domain numerical approach for solving Maxwell's equations of electrodynamics. The FDTD method was first introduced by Kane Yee in 1966 [1], and has become increasingly popular in the electromagnetic modeling and simulation community as available computational resources have expanded.

The general Yee FDTD algorithm staggers the E and H-field vector components within a cubical lattice. The grid is created in such a way so that each E-field component is surrounded by four H-field components and each H-field component is surrounded by four E-field components, as shown in the following figure.

The Yee algorithm also staggers the E and H-field components in time, so that they are updated in a leapfrog manner. The current value of an E-field at a point is calculated based on the previous value of the E-field at that point and from the previously stored values of the four encircling H-fields. Next, the H-fields are updated using the previous H-field values and the four encircling E-fields. This process is repeated until the desired solution state has been reached.

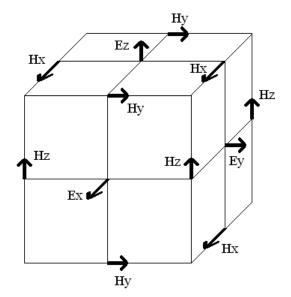


Figure 1

FDTD Update Equations:

Maxwell's equations for linear, isotropic, nondispersive, lossy materials can be written as:

$$\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu} \nabla \times \vec{E} - \frac{1}{\mu} \mathbf{Q}_{source} + \sigma^* \vec{H}$$

$$\frac{\partial \vec{E}}{\partial t} = \frac{1}{\varepsilon} \nabla \times \vec{H} - \frac{1}{\varepsilon} \left(\int_{\text{source}} + \sigma \vec{E} \right)$$

These equations may be vectorized and written in terms of their Cartesian coordinate components. For example, the x-directed component equations become:

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left[\frac{\partial E_y}{\partial z} - \frac{\partial Ez}{\partial y} - \mathbf{M}_{source-x} + \sigma^* H_x \right]$$

$$\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon} \left[\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \mathbf{q}_{source-y} + \sigma E_x \right]$$

Applying Yee's finite difference scheme, and rearranging terms, the FDTD update equations for the x-directed E and H-field components may be written as:

$$E_{x}\Big|_{i,j,k}^{n+1/2} = \left(\frac{1 - \frac{\sigma_{i,j,k}\Delta t}{2\varepsilon_{i,j,k}}}{1 + \frac{\sigma_{i,j,k}\Delta t}{2\varepsilon_{i,j,k}}}\right) E_{x}\Big|_{i,j,k}^{n-1/2} + \left(\frac{\frac{\Delta t}{\varepsilon_{i,j,k}}}{1 + \frac{\sigma_{i,j,k}\Delta t}{2\varepsilon_{i,j,k}}}\right) \cdot \left(-\frac{H_{z}\Big|_{i,j+1/2,k}^{n} - H_{z}\Big|_{i,j-1/2,k}^{n}}{\Delta z} - \frac{H_{z}\Big|_{i,j+1/2,k}^{n} - H_{z}\Big|_{i,j-1/2,k}^{n}}{\Delta z} - \frac{\Delta z}{-J_{source-x}\Big|_{i,j,k}^{n}}\right)$$

$$H_{x}\Big|_{i,j,k}^{n+1} = \left(\frac{1 - \frac{\sigma_{i,j,k}^{*} \Delta t}{2\mu_{i,j,k}}}{1 + \frac{\sigma_{i,j,k}^{*} \Delta t}{2\mu_{i,j,k}}}\right) H_{x}\Big|_{i,j,k}^{n} + \left(\frac{\frac{\Delta t}{\mu_{i,j,k}}}{1 + \frac{\sigma_{i,j,k}^{*} \Delta t}{2\mu_{i,j,k}}}\right) \cdot \frac{\left[\frac{E_{y}\Big|_{i,j,k+1/2}^{n+1/2} - E_{y}\Big|_{i,j,k-1/2}^{n+1/2}}{\Delta z}\right]}{\Delta z} - \frac{E_{z}\Big|_{i,j+1/2,k}^{n+1/2} - E_{z}\Big|_{i,j-1/2,k}^{n+1/2}}{\Delta y} - \frac{\Delta y}{\Delta y} - M_{source-x}\Big|_{i,j,k}^{n+1/2}$$

The y and z-directed update equations can be written in a similar manner.

SAR Calculations:

The Specific Absorption Rate (SAR) is commonly used as a measure of the energy absorption within biological tissues. The SAR can be calculated by

$$\frac{\sigma |E|^2}{
ho}$$

where ρ is the density in Kg per cubic meter, σ is the conductivity, and E is the root-mean-square of the total Electric field.

For sinusoidal steady-state calculations, the FDTD update equations are typically iterated until the SAR has reached an acceptable convergence criteria.

Boundary Conditions

Absorbing Boundary Conditions (ABC) are often used with the Finite Difference Time Domain (FDTD) method in order to simulate the extension of the computational zone to infinity. This is necessary in order to properly predict the electromagnetic fields within an unbounded region. In the past, analytical techniques have been used to achieve the absorbing boundary condition. More recently, the Perfectly Matched Layer (PML) boundary condition has been introduced and favored in many FDTD simulations. The PML is an absorbing material medium that ideally will match plane waves of any incidence angle, polarization, or frequency.

In the main computational space of an FDTD grid, E-field and H-field update equations are performed in a leapfrog manner in order to calculate the electromagnetic fields at the current time step. Within a PML boundary layer, in addition to the E-field and H-field updates, the electric flux density (D) and the magnetic flux density (B) are required. The update equations for the x-directed electromagnetic components within the PML boundary are given below. Similar equations apply for the y-directed and z-directed components.

$$D_{x}\Big|_{i,j,k}^{n+1} = \left(\frac{2\varepsilon\kappa_{y} - \sigma_{y}\Delta t}{2\varepsilon\kappa_{y} + \sigma_{y}\Delta t}\right)D_{x}\Big|_{i,j,k}^{n} + \left(\frac{2\varepsilon\Delta t}{2\varepsilon\kappa_{y} + \sigma_{y}\Delta t}\right) * \left[\frac{H_{z}\Big|_{i,j+1/2,k}^{n+1/2} - H_{z}\Big|_{i,j-1/2,k}^{n+1/2}}{\Delta y} - \frac{H_{y}\Big|_{i,j,k+1/2}^{n+1/2} - H_{z}\Big|_{i,j,k-1/2}^{n+1/2}}{\Delta z}\right]$$

$$E_{x}\Big|_{i,j,k}^{n+1} = \left(\frac{2\varepsilon\kappa_{z} - \sigma_{z}\Delta t}{2\varepsilon\kappa_{z} + \sigma_{z}\Delta t}\right) E_{x}\Big|_{i,j,k}^{n} + \left(\frac{1}{\mathbf{Q}\varepsilon\kappa_{z} + \sigma_{z}\Delta t}\right) * \mathbf{E}\varepsilon\kappa_{x} + \sigma_{x}\Delta t \mathcal{D}_{x}\Big|_{i,j,k}^{n+1} - \mathbf{Q}\varepsilon\kappa_{x} - \sigma_{x}\Delta t \mathcal{D}_{x}\Big|_{i,j,k}^{n}$$

$$B_{\boldsymbol{x}}\big|_{i,j,k}^{n+3/2} = \left(\frac{2\varepsilon\kappa_{\boldsymbol{y}} - \sigma_{\boldsymbol{y}}\Delta t}{2\varepsilon\kappa_{\boldsymbol{y}} + \sigma_{\boldsymbol{y}}\Delta t}\right) B_{\boldsymbol{x}}\big|_{i,j,k}^{n+1/2} - \left(\frac{2\varepsilon\Delta t}{2\varepsilon\kappa_{\boldsymbol{y}} + \sigma_{\boldsymbol{y}}\Delta t}\right) * \left[\frac{E_{\boldsymbol{z}}\big|_{i,j+1/2,k}^{n+1} - E_{\boldsymbol{z}}\big|_{i,j-1/2,k}^{n+1}}{\Delta \boldsymbol{y}} - \frac{E_{\boldsymbol{y}}\big|_{i,j,k+1/2}^{n+1} - E_{\boldsymbol{z}}\big|_{i,j,k-1/2}^{n+1}}{\Delta \boldsymbol{z}}\right]$$

$$H_{x}\Big|_{i,j,k}^{n+3/2} = \left(\frac{2\varepsilon\kappa_{z} - \sigma_{z}\Delta t}{2\varepsilon\kappa_{z} + \sigma_{z}\Delta t}\right) H_{x}\Big|_{i,j,k}^{n+1/2} + \left(\frac{1}{\sqrt{\varepsilon\kappa_{z} + \sigma_{z}\Delta t}}\right) * \left[\!\!\!\left\{\varepsilon\kappa_{x} + \sigma_{x}\Delta t\right\}\!\!\!\right]_{x}\Big|_{i,j,k}^{n+3/2} - \sqrt{\varepsilon\kappa_{x} - \sigma_{x}\Delta t}\right] H_{x}\Big|_{i,j,k}^{n+1/2} = \left(\frac{1}{\sqrt{\varepsilon\kappa_{z} + \sigma_{z}\Delta t}}\right) + \left(\frac{1}{\sqrt{\varepsilon\kappa_{z} + \sigma_{z}\Delta t$$

A polynomial profile is applied to the σ and κ terms within the PML in order to reduce reflections caused by discretization errors. The value of these coefficients may be calculated at a given depth within the PML based on the following equations.

$$\sigma_{x}(x) = \sqrt[4]{d} \sigma_{x,\text{max}}$$

$$\kappa_{x}(x) = 1 + \left(\kappa_{x, \text{max}} - 1 \right) \left(\kappa_{d} \right)$$

In equations 5 and 6, d is the depth from the PML surface. The polynomial factor m is typically given a value between 3 and 4. For a given value of m, $\sigma_{x,max}$ can be calculated by the following equation, whereas $K_{x,max}$ is often just set to 1 within the PML.

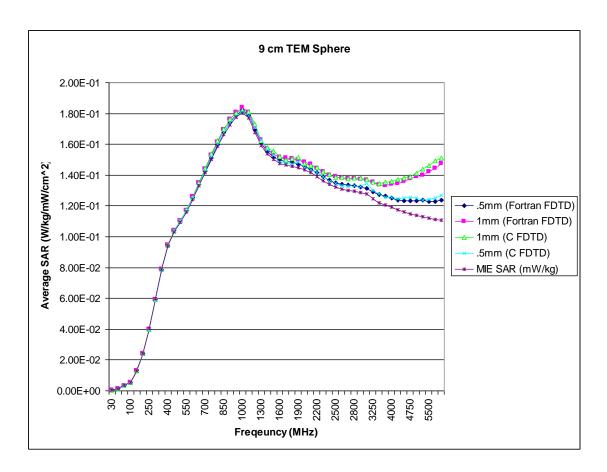
$$\sigma_{x,\text{max}} = \frac{0.8(m+1)}{\eta \Delta}$$

A complete derivation and description of the implementation of a PML boundary can be found in Taflove pages 298-313 [6].

Results and Discussion

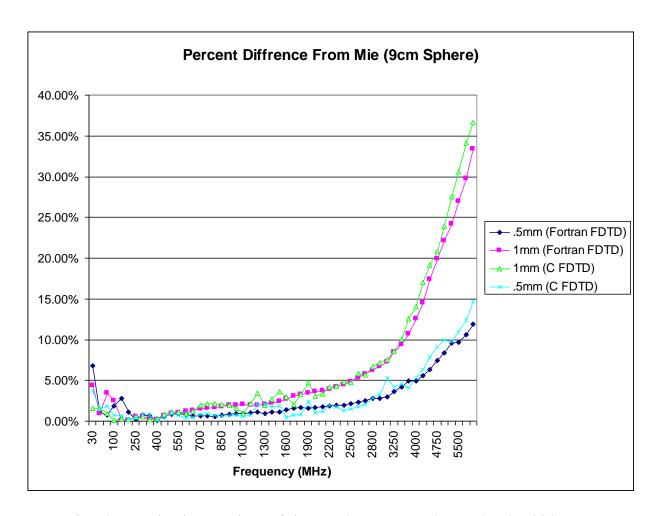
Brooks FDTD, especially the Fortran version, has been validated using many different methods including: exact analytical solutions of simple geometries, comparisons against other numerical methods for EM, comparisons against other validated FDTD codes, and even traditional empirical experiments. For validation purposes of this technical report, we compare both Brooks FDTD implementations (FORTRAN and C) against a Mie theory based code.

In our test setup, we consider a 9cm sphere made of a tissue equivalent material (TEM) being exposed to a plane wave ranging in frequency from 30 MHz to 6 GHz. In our FDTD runs, we will use both 1mm and 0.5mm resolution spheres. The following chart depicts the FDTD and Mie results in terms of whole body SAR:

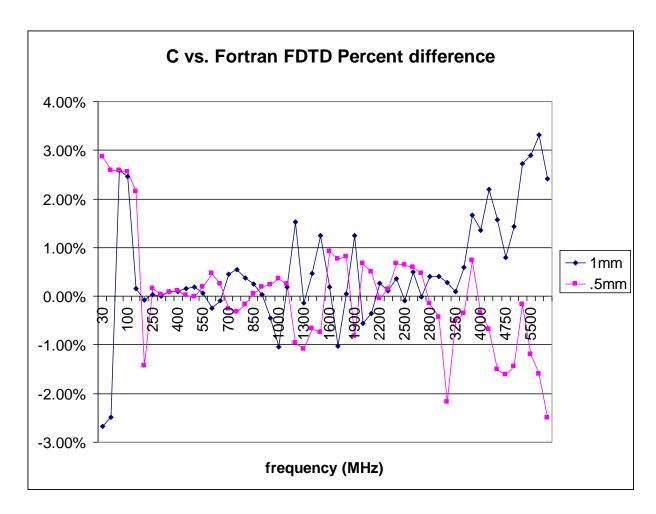


The chart shows a tight correlation between the two implementations for lower frequencies, but as the frequencies increase, FDTD starts to diverge. It is well know that the FDTD method breaks down as the voxel size becomes large as compared to the frequency of the incident field [5]. Generally, at least 10 cells per wavelength are recommended for accurate results.

Using the 10 cells per wavelength requirement, the 1mm sphere model and the 0.5mm sphere model would be appropriate for frequencies up to 3.6 GHz and 7.6 GHz, respectively. In this case, these upper bounds have errors of \sim 10% compared to the MIE solution. If better accuracy is required, higher resolution models would be advised.



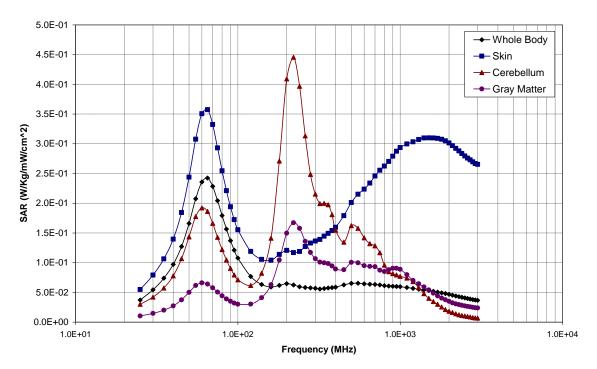
Comparing the two implementations of the Brooks FDTD code, results should be very close as the algorithms are almost identical. Minor deviations in their results would be primarily due to differences in compilers and math libraries. The following chart plots the percent differences between the results of the C and Fortran versions:



Differences between the C and Fortran implementations of Brooks FDTD rarely exceed 1% where FDTD is known to be stable.

The main benefit between FDTD and exact solutions like the Mie method is that FDTD can run arbitrary geometries. The following are SAR results from the Fortran version of the Brooks FDTD code. In these simulations, RF fields with frequencies from 25 MHz to 3 GHz were incident dorsally upon a 1mm anatomical man model. Vertical electric field polarization was assumed for the incident field. The graph below depicts SAR in a handful of tissues as a function of frequency.

1mm Man MEHK



The chart shows just a portion of the tissues found in the 1mm anatomical man model. Brooks FDTD produces a full SAR output for every 1mm voxel of the model. These results can be visualized by any number of tools.

CONCLUSIONS

The Brooks FDTD FORTRAN and C codes were observed to match the Mie values with a very small margin of error of 5% for frequencies between 30 MHz and 2.5 GHz for 1mm resolution models and between 30 MHz and 4 GHz for 0.5 mm resolution models. The Brooks FDTD codes had a margin of error that grew as the frequencies moved above these ranges and generally could not produce reliable results when the wavelength is shorter than 10 cells. For higher frequencies beyond 7.6 GHz, FDTD can still be employed, but models at a higher resolution than 0.5 mm are required for accurate results.

FDTD has been proven to be a valuable tool for modeling RF bioeffects. With increasing computing capacity, FDTD can be taken even further in the future with larger and higher resolution models of arbitrary geometries. Modeling with FDTD allows researchers to simulate hundreds or even thousands of scenarios before any empirical experimentation begins. Brooks FDTD continues to be developed and maintained to ensure accuracy and to provide useful features for continued RF bioeffects research.

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Appendix A: Brooks FDTD Fortran Source

The source code is included on accompanying CD under the "src/fortran_version" directory.

Appendix B: Brooks FDTD (Fortran Based) User Guide

Install Procedures

Assumptions

- Compatible Fortran 95 compiler
- Working MPI environment
- /usr/local is exported to all nodes in the cluster
- The MPI libraries and Fortran library paths are in the load search path or are in the "LD LIBIRARY PATH" environment variable
- Name the MPI Fortran 90/95 wrapper compiler "mpif90"
- Log in as root

Building Brooks FDTD

- 1. Uncompress the FDTD source files into a temporary directory
- 2. In that directory, type "make"
- 3. Copy the "fdtd" binary to /usr/local/bin, and make sure permissions are set to 555 or higher
- 4. Temporary directory and files may be deleted

How to Run FDTD Simulations

Introduction

Assuming you have configured your cluster and compiled the code properly, running the code is relatively simple. Generally most problems running the code stem from cluster misconfigurations. This guide will step you through running sample problems.

Overview

- 1. Command Synopsis
- 2. Options Description
- 3. Required Files
- 4. RF Source Cardinal Polarizations for plane wave

Command Synopsis

```
mpirun [mpi options here] fdtd < model.dat -ifile
antenna.dat -t tissue.txt
[-air n_layers] [-r] [-v string] [-eout] [-hout] [-t
[grid|id]] [-i nbytes] [-ps] [-pml] [?]</pre>
```

Options Description

<pre>? < model.dat (required)</pre>	Prints usage Okay, this is not really an option, but redirection of stdin; still, it is necessary none the less. "model.dat" contains the information about the model on which you are running the simulation. Refer to the required files section for more information as to what goes in to model.dat, and all other required files.
<pre>-ifile antenna.dat (required)</pre>	Specifies incident field file or antenna file. The antenna dat file contains information describing the RF source. For this version, the two source options are point source, and plane wave.
-tfile tissue.txt	Specifies the tissue file that relates to the model included.
<pre>(required) -air n_layers</pre>	Adds n extra layers of air around the model. For example, if n equals 3 and your model is (21, 21, 21) voxels^3, then the new total size would be (27, 27, 27). No less than 10 layers of air should be used. If the -pml option is not used, additional layers may be required depending on the
-r	frequency. Forces root to calculate.
-v string	Allows "string" to be appended to the file prefixes
-eout	Outputs the E-field values in x, y, and z at the end of the simulation.
-hout	Outputs the H-field values in x, y, and z at the end of the simulation.
-t [grid id]	Unsuppressed troubleshooting output. "grid" will print the "gridMap" assignments, and "id" will create an output file.
-i n_bytes	Preallocates n_bytes of memory for the incident field.
-maxe	Creates an output file that contains the maximum e value for each cell during a run
-ps	Specifies the simulation will be of a point source, and not a plane wave. The point source configuration file must included with the –ifile option
-pml	Specifies that an eight layer PML absorbing boundary condition (ABC) is to be used instead of the regular one layer ABC.

Required Files

The '#' characters and following text are included in the examples only for descriptive purposes, and should not be included in you actual files. Not all routines were written to handle comments, and some fields are hard coded to read in a fixed amount number of characters.

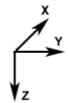
model.dat

Describes	the	model	and	the	frequencies	to	be	run.			
tissue.txt	#Name	e of tissu	ae prop	erties	file to be used	l					
./	#Out	#Output Directory Dirpre									
Test	#Out	out file p	prefix.	This w	ill be prepende	ed to	all ou	tput			
.05	#Cut	off for ra	atio di	ff from	1.0		crit				
4	#Min:	imum numbe	er of h	alf cyc	les to run		minhc	ус			
10	#Min	Time step	os per	wavelen	gth		dtper	wave			
Testrawfile	e.raw	#Model :	file				rawfi	le			
10	#The	X Dimens	ion of	the Mod	el Orientation		nx				
10	#The	Y Dimens	ion of	the Mod	el Orientation		ny				
10	#The	Z Dimens	ion of	the Mod	el Orientation		nz				
0.002	#Vox	el size in	n X in 1	meters							
0.002	#Vox	el size in	n Y in 1	meters							
0.002	#Vox	el size in	n Z in 1	meters							
2060.	#Fre	quency in	MHz								
3000.	#Mul	tiple fred	quencie	s can b	e listed here						

used. The following types of antenna/sources are available with this version of FDTD: point source and plane wave.

antenna.dat for plane wave

The vector to the plane wave source is found using the theta and phi method. Imagine yourself in the x-z plane with your feet in the +z direction, and your left side in the +x direction. Take your right arm and rotate it from -z to +z in the x-z plane for theta. Next, rotate your arm counter-clockwise for the phi. For example if your vector is theta=90, and phi=90, the vector would first rotate from -z to -x for theta=90, then it would rotate from -x to +y for phi. The result is a vector going in the +y direction.



(90.0 0.0 1.0 0.0	<pre>#Theta latitude (degrees) #Phi longitude (degrees) #E theta #E phi #Magnitude</pre>	thinc phinc ethinc epthinc
-	1.0	#Magnitude	-

antenna.dat for point source (sinusoidal)

	1 /
50	<pre>#x location of ps</pre>
100	#y location of ps
500	#z location of ps
1.0	#Amplitude
1	#Orientation
0	<pre>#ps type (0 == sinusoidal, 1 == Gaussian pulse)</pre>

antenna.dat for point source (Gaussian pulse)

```
50
                   #x location of ps
100
                   #y location of ps
500
                   #z location of ps
1.0
                   #Amplitude
                   #Orientation
1
                   #ps type (0 == sinusoidal, 1 == Gaussian pulse)
1
200.0
                   #n sub 0
50.0
                   #n decay
```

Defines the dielectric properties of the tissue types found in the raw file.

lues are as

1.

- 2. Label
- 3. R of the RGB value
- 4. G of the RGB value
- 5. B of the RGB value
- 6. Density (only used for SAR calculations)
- 7. Epsilon infinity
- 8. del1
- 9. 1/(2pi * tau1)
- 10. (1-alf1)
- 11. del2
- 12. 1/(2 pi * tau2)
- 13. (1-alf2)
- 14. del3
- 15. 1/(2pi * tau3)
- 16. (1-alf3)
- 17. del4
- 18. 1/(2pi * tau4)
- 19. (1-alf4)
- $20. \sigma_i$
- 21. ID Number

Where, $\varepsilon_0 = 8.854*10^{-12}$ and $\omega = 2*pi*freq$, Re lative Permittivity = Re al ε ω \square , Conductivity = $2*\pi*eps_0*freq*imaginary$ ε ω \square and,

$$\varepsilon \boxtimes \omega \vDash \varepsilon_{\infty} \Box \frac{del_{1}}{1 \Box \Box j \omega \tau_{1}} \Box \frac{del_{2}}{1 \Box \Box j \omega \tau_{2}} \Box \frac{del_{3}}{1 \Box \Box j \omega \tau_{3}} \Box \frac{del_{4}}{1 \Box \Box j \omega \tau_{4}} \Box \sigma_{i} / j \omega \varepsilon_{0}$$

RF Source Cardinal Polarizations for Plane Wave

	FDTD Parameters						Anatomical Orientation		
Polarization	Theta	Phi	ThetaPolar	PhiPolar	Head /	Right	Front		
					Tail	/ Left	/ Back		
PEHK	90	90	1	0	Е	Н	F>B		
MEHK	90	270	1	0	E	Н	B>F		
PEKH	90	0	1	0	E	L>R	Н		
MEKH	90	180	1	0	E	R>L	Н		
PHEK	90	90	0	1	Н	E	F>B		
MHEK	90	270	0	1	Н	E	B>F		
PHKE	90	0	0	1	Н	L>R	E		
MHKE	90	180	0	1	Н	R>L	E		
PKEH	0	0	1	0	H>T	E	Н		
MKEH	180	0	1	0	T>H	Е	Н		
PKHE	0	0	0	1	H>T	Н	E		
MKHE	180	0	0	1	T>H	Н	Е		

K is listed by H>T, T>H, L>R, R>L, F>B, or B>F where H means head, T tail, L left, R Right, F front, and B back. These are meant to signify the direction of K; for example, H>T means head to tail. Front refers to the human front, or anatomically the ventral side. There is not a single unique combination of parameters for each orientation, and the program will accept other parameters including values between 0.0, and 1.0 for ThetaPolar, and PhiPolar, but all values have not been tested, so be careful. Assumptions: x is side to side, y is front to back, and z is head to tail.

Appendix C: Brooks FDTD C Source

The source code is included on accompanying CD under the "src/c_version" directory.

Appendix D: Brooks FDTD (C Based) User Guide

Installing FDTD:

Compiling FDTD should be a simple affair assuming a C compiler, MPI libraries, and a properly configured environment. This FDTD implementation has been compiled without problems with GCC gcc 4*, Intel icc 8-10, and PGI pgcc 6-7 with MPI implementations from LAM-MPI, OpenMPI, and Cray.

To compile FDTD with the Makefile, type in the directory of the source code:

```
$ make
```

To compile FDTD without the Makefile, type:

```
$ mpicc -o fdtd *.c -lz -lm -lrt -O3
```

To install FDTD, simply copy the binary to anywhere that is in your path and is accessible to all the nodes on your cluster. For example, if /usr/local is exported to all nodes, you could copy the binary to /usr/local/bin, or if you don't have access to copy it there, you can copy it to your own personal ~/bin directory.

```
# cp ./fdtd /usr/local/bin
-or-
$ cp ./fdtd ~/bin
```

Input:

Most of FDTD's features are controllable through command line options.

Command Line Options:

Options Always Required:

- --raw/-r [raw file name]
 - o The main model file that simulation will run against
- --freg/-f [frequency]
 - Used to calculate the dielectric properties of the tissue types
 - Used for the source if it requires a frequency
- --tissue/-t [tissue file name]
 - o Tissue/material properties file

Options Required for a Plane Wave Incident Field:

- --pw/-P [theta,phi,theta_amp,phi_amp]
 - o A file name with the same parameters one per line is also acceptable

Additional Options

• --air/-a [number of air layers]

- o If unspecified, 10 layers of air are added on by default
- o It is not recommended to have less than 1 layer of air
- --delta/-d [dx,dy,dz]
 - o specifies the cell size in meters
 - o Default cell size values are 0.001,0.001,0.001 m
- --maxe/-m
 - Tracks the maximum E-field values and produces a SAR like file for all cells in the model
- --pml/-p [number of PML layers]
 - o Default number of PML layers is 8
 - o Less than 4 layers is not recommended, and less than 1 will not work.
- --prefix/-x [output prefix]
 - o Provides the prefix for the output files
 - o The default prefix is the raw file name minus the ".raw" ending
- --iterations/-i [max number of iterations]
 - o The maximum number of iterations or time steps to run
- --logfile/-l [log file name]
 - o Defaults to [prefix].log
- --verbose/-v
 - More output to the shell
- --help/-h/-?
 - o Prints out usage

RAW File:

The RAW file contains the model or geometry. It is 3D volumetric data stored as a 1D binary stream of bytes/chars. Each byte cast to an unsigned integer corresponds to one of the possible 256 tissue type IDs found in the tissue file. The 1D stream is organized in increasing order first in the x, then y, and finally z directions. Files of this format can be read and written with the following algorithm:

FDTD expects the filename to contain the dimensions of the file in the following format: x[interger]y[integer]z[integer].raw. For example, a file named "sphere x0101y0101z0101.raw" would specify the mode to be 101x101x101 cells.

Tissue File:

The tissue file contains the dielectric properties of all of the materials found in the raw file. The file is organized with 20 comma separated columns and a row per tissue type. The columns in order are:

1. Material name 2. R (red) 3. G (green) 4. B (blue) 5. specific density 6. ε_{∞} or infinite dielectric value 8. f_1 or dispersion frequency 1 9. α_1 10. $\Delta \epsilon_2$ 11. f_2 or dispersion frequency 2 12. α_2 13. $\Delta \epsilon_3$ 14. f_3 or dispersion frequency 3 15. α_3 16. Δε₄ 17. f_4 or dispersion frequency 4 18. α_4 19. σ_0 or DC conductivity 20. Tissue ID

Output

FDTD outputs several files: specific absorption rate (SAR), log file, and maximum E-field file if the --maxe options was used. The sar and maxe 3D volumetric data as a 1D binary stream of floats organized in the same way as the raw file.

Running FDTD

FDTD was designed to be executed in parallel on a Beowulf type cluster, but anything with a C compiler and a MPI implementation should work.

Basic execution of FDTD:

```
mpirun [mpi options] fdtd [fdtd options]
```

The following is an example of how to run a plane wave on a sphere on 2 processors:

```
mpirun -np 2 fdtd -r Sphere_x0021y0021z0021.raw -t
tissue.txt -f 3000 -P 90,0,1,0 -v
```

Example Torque script to submit a FDTD run to a Torque/PBS based resource management system:

```
#!/bin/bash
#PBS -l nodes=2:ppn=2

mpirun fdtd -t tissue.txt -r sphere_x0120y0120z0120.raw -v
-f 500 --pw 90,0,1,0 -l test_log.out -a 10 --prefix job_8
exit 0
```

Appendix E: Model Files

The model files are included on accompanying CD under the "models" directory. Model files are stored in the RAW format as discussed in Appendix D under the heading "RAW Files." Generally the file name describes what the RAW file is; for example, man_lmm_x0586y0340z1878.raw specifies the visible man at a 1mm resolution. Typically if no resolution is specified, 1mm is assumed. The corresponding dielectric properties for each model voxel is located in "/models/tissue.txt".